

Mott insulators and correlated superfluids in ultracold Bose-Fermi mixtures

F. Hébert¹, F. Haudin¹, L. Pollet,² and G.G. Batrouni¹

¹INLN, Université de Nice-Sophia Antipolis, CNRS; 1361 route des Lucioles, 06560 Valbonne, France and

²Institut für Theoretische Physik, ETH Zürich, CH-8093, Switzerland

We study the effects of interaction between bosons and fermions in a Bose-Fermi mixtures loaded in an optical lattice. We concentrate on the destruction of a bosonic Mott phase driven by repulsive interaction between bosons and fermions. Once the Mott phase is destroyed, the system enters a superfluid phase where the movements of bosons and fermions are correlated. We show that this phase has simultaneously correlations reminiscent of a conventional superfluid and of a pseudo-spin density wave order.

PACS numbers: 05.30.Jp, 03.75.Hh, 71.10.Fd, 02.70.Uu

Cold atoms loaded on optical lattices provide a new tool to study condensed matter systems. These systems are experimental realizations of lattice models for quantum interacting particles such as Hubbard models. They provide a simple and controllable way to study various interesting phenomena such as the superfluid to Mott insulator (MI) transition [1] or Anderson localization [2]. Recently, there has been growing interest in the physics of boson-fermion mixtures at low temperature. These mixtures served originally to lower the temperature of the fermions by sympathetic cooling [3] with the bosons in order to study the low temperature physics of interacting fermions, such as superfluidity in the BCS or BEC regime [4].

In some cases the interactions between fermions and bosons cannot be neglected. Fermions have, for example, been shown to reduce the phase coherence of weakly interacting superfluid bosons [5]. Theoretical studies [6, 7, 8] have suggested the possibility for the system to form pairs (polarons) of bosons and fermions (particle-particle or particle-hole), with these composite fermionic pairs then adopting different phases such as normal Fermi liquid or solid phases. This system was studied numerically in one dimension by Sengupta et Pryadko [9] and shows a commensurate filling phase where the sum of the number of bosons, N_b , and fermions, N_f , is equal to the number of lattice sites L : $N_b + N_f = L$. This phase has been studied simultaneously in the special case where $N_b = N_f = L/2$ by Pollet *et al.* [10] who showed that it could be understood, in the strong interaction limit, as the pseudo-spin density wave (PSDW) phase previously proposed by Kuklov and Svistunov [6]. This kind of system has also been studied in the presence of harmonic traps [11], but the comparison with experiment [5] is problematic.

In this letter we study the effect of added fermions on a bosonic MI phase [1] at low temperature. As the boson-fermion interaction is increased, the MI is destroyed and the system enters a superfluid phase (SF). We will review the properties of this phase and show that it can be crudely described as composed of superfluid bosons and of the aboved mentioned PSDW phase. In addition, we

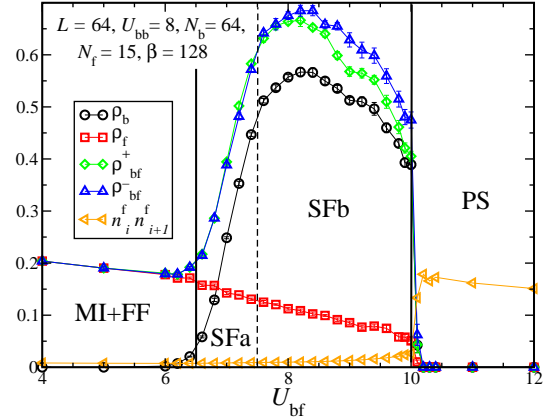


FIG. 1: At low U_{bf} , the system consists of free fermions on a bosonic Mott insulator substrate. As U_{bf} becomes larger the Mott insulator is destroyed and the system becomes superfluid (SF). There is a crossover between two different superfluid regions (see the text). Finally for large values of U_{bf} , fermions and bosons phase separate (PS).

study the properties of the PSDW phase when there is an imbalance in the boson and fermion populations but with $N_b + N_f = L$.

The system is described by a one-dimensional repulsive Hubbard model

$$\mathcal{H} = -t \sum_i \left(b_i^\dagger b_{i+1} + f_i^\dagger f_{i+1} + \text{h.c.} \right) + U_{bb} \sum_i n_i^b (n_i^b - 1)/2 + U_{bf} \sum_i n_i^b n_i^f, \quad (1)$$

where the operator b_i^\dagger (b_i) creates (destroys) a boson on site i while f_i^\dagger and f_i are the corresponding fermionic operators. The first term in (1) describes the hopping of bosons and fermions between neighboring sites. We have chosen the hopping amplitude $t = 1$, which sets the energy scale, to be the same for both species. n_i^b (n_i^f) is the bosonic (fermionic) number operator at site i and U_{bb} and U_{bf} are the boson-boson and boson-fermion contact interaction terms.

The bosonic, $G_b(x) = \langle b_i^\dagger b_{i+x} \rangle$, fermionic, $G_f(x) =$

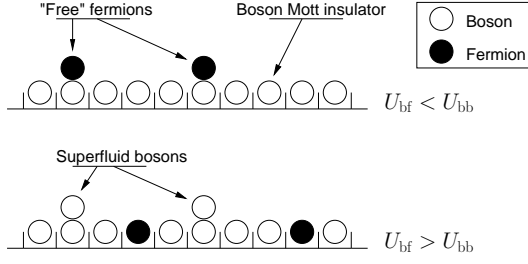


FIG. 2: Schematic representation of the destruction of the bosonic Mott insulator. As U_{bf} is increased, the sites that were occupied by a boson and a fermion are replaced by sites occupied by two bosons. The number of bosons per site is no longer 1 and the system can become superfluid.

$\langle f_i^\dagger f_{i+x} \rangle$, and composite, $G_{bf}(x) = \langle b_i^\dagger f_{i+x}^\dagger b_{i+x} f_i \rangle$, Green functions, give access to the phase correlations of bosons, fermions and particle-hole pairs, respectively. A non vanishing bosonic superfluid density $\rho_b = \langle W_b^2 \rangle / 2\beta$ or a fermionic stiffness $\rho_f = \langle W_f^2 \rangle / 2\beta$ shows the presence of slowly (algebraically) decaying phase correlations (W_b and W_f being the bosonic and fermionic winding numbers). The paired (+) and counter-rotating (-) superfluid densities, $\rho_{bf}^\pm = \langle (W_b \pm W_f)^2 \rangle / 2\beta$ are both equal to $\rho_b + \rho_f$ if the movements of the two types of particles are uncorrelated and differ if the movements are correlated (or anticorrelated).

We study this model using a canonical quantum Monte Carlo method based on “worm” updates which is extremely efficient for the measurements of equal time Green functions [12]. This method was modified to tackle the case of mixtures by allowing simultaneous moves of the bosons and fermions [13].

We set the number of bosons N_b to be equal to the number of sites $L = 64$ and set $U_{bb} = 8$, to obtain a solid Mott phase for the bosons in absence of interactions with the fermions. We studied the evolution of the system as U_{bf} is gradually increased for two different values of the number of fermions ($N_f = 15$ and 35).

For $U_{bf} < 6.5$ the superfluid densities (Fig. 1) show that the system behaves as in the non interacting limit (MI+FF). The bosons form a MI where $\rho_b = 0$, each site is occupied by only one boson and jumps are forbidden because they cost a large energy U_{bb} . On the contrary, the fermions move freely as they experience the same interaction energy U_{bf} on all the sites ($\rho_f \neq 0$). When U_{bf} becomes larger than U_{bb} the Mott insulator is destroyed and the bosons become superfluid. In this case, it is energetically favorable to form pairs of bosons on the same site and to have isolated fermions (Fig. 2). The system is then split into doped superfluid bosonic regions and fermions. If the repulsion between bosons and fermions is not too strong ($6.5 < U_{bf} < 10$), the bosons can pass from one superfluid region to the next one by the tunnelling through fermion-occupied sites and a superfluid

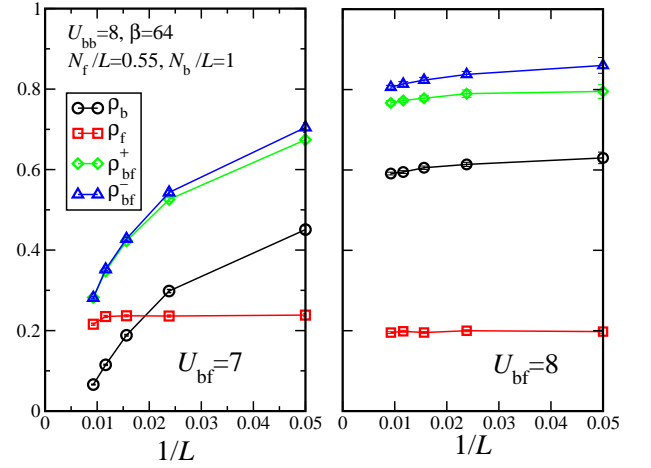


FIG. 3: Finite size scaling of different densities for two values of the interaction. The SFa regime observed in Fig. 1 around $U_{bf} \simeq 7$ disappears for larger size whereas the SFb regime persists for $U_{bf} \simeq 8$.

(SF) phase is established. For $U_{bf} > 10$ the tunnelling is suppressed and there is a phase separation between independent superfluid regions separated by fermionic regions. This case is difficult to study numerically because the system is frozen.

When the MI is destroyed, two distinct regions [14], separated by a crossover, appear: a first region (SFa, $6.5 < U_{bf} < 7.5$) where correlations of the movements of bosons and fermions are not visible ($\rho_b + \rho_f = \rho_{bf}^\pm$) and a second one (SFb, $7.5 < U_{bf} < 10$) where $\rho_{bf}^- > \rho_{bf}^+$. In this latter region moving a fermion independently of the surrounding bosons costs U_{bf} , while exchanging a boson and a fermion has no energy gap associated. These favored exchanges lead to the observed anticorrelation of winding numbers.

The SFa region disappears in the thermodynamic limit (or at least becomes very narrow) as can be observed in Fig. 3, where ρ_b goes to zero with $1/L$ for $U_{bf} = 7$. On the contrary, around $U_{bf} = 8$, the SFb phase persists in the large size limit. We then expect a direct transition from the MI+FF phase to the SFb regime (Fig. 3 corresponds to a density of fermions $N_f/L \simeq 0.55$ but the two values of U_{bf} correspond to the same phases as in Fig. 1 where $N_f/L \simeq 0.23$).

In Fig. 4, we show the Green functions in the MM+FF (left) and in the SFb (right) phases. In the Mott phase, $G_b(x)$ decays exponentially while $G_f(x)$ decays algebraically following the free fermion Green function $G_f(x) = \sin(N_f \pi x / L) / \sin(\pi x / L)$. The two species are independent, in spite of the large value of U_{bf} , and consequently $G_{bf} = G_b G_f$.

In the SFb, all the Green functions decay algebraically. The slowest decay is obtained for the bosons with $G_b \propto \sin(\pi x / L)^{-0.35}$ while $G_f \propto \sin(N_f \pi x / L) \cdot \sin(\pi x / L)^{-1.5}$. In this case, G_{bf} is much larger than both the product

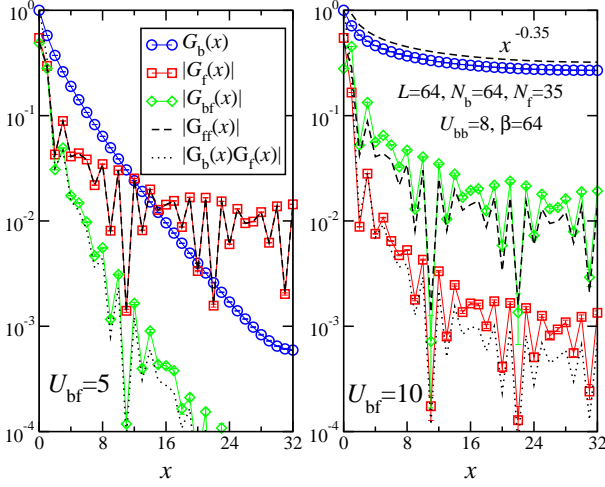


FIG. 4: Left : For $U_{bf} = 5$ the bosons are in a Mott insulating state and G_b decays exponentially. The fermions follow the free fermions behavior. Right: In SFb regime, we observe phase coherence in all the cases. G_{bf} is larger than G_f .

$G_b G_f$ and G_f and follows (approximately) G_{ff} . This behavior confirms that boson-fermion pairs are important degrees of freedom in this system (in the SFa region, on the contrary, G_f is larger than G_{bf} [14]).

Returning to Fig. 2, an intuitive but crude physical interpretation is, that our system can be roughly described as composed of N_f superfluid bosons and a layer composed of N_f fermions and $L - N_f$ bosons. For such a “filled” layer, the description of the system as pseudo-spins is possible [6, 10] whose properties we now review. Once again, we concentrate on the case where the bosons are strongly interacting ($U_{bb} = 8$) and all the cases where $N_f + N_b = L$. First, for small U_{bf} , the full system is composed of two weakly interacting Luttinger liquids, one for each species. Green functions decay algebraically (Fig. 5, $U_{bf} \leq 2$) and the winding numbers W_b and W_f are not correlated (Fig. 6, left).

For large enough U_{bf} the system enters a PSDW phase: The interactions forbid double occupancy of a site by two bosons or by a fermion-boson pair and a pseudo-spin along the z -axis on site i may be defined as $\sigma_i^z = n_i^b - n_i^f = \pm 1$. The model can then be mapped on the XXZ Hamiltonian

$$\mathcal{H}_{XXZ} = J_{xy} (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y) + J_z \sigma_i^z \sigma_{i+1}^z$$

where $J_{xy} = -t^2/U_{bf}$ and $J_z = t^2(1/U_{bf} - 1/U_{bb})$. The magnetic correlations along the xy axes correspond to particle-hole correlations $G_{bf}(x)$ as $\sigma_i^+ \propto b_i^\dagger f_i$. Bosonic and fermionic Green functions decay exponentially as the hopping of individual particles is energetically suppressed (Fig. 5, $U_{bf} \geq 3$). The hopping of bosons and fermions and, consequently, the winding numbers are strongly anti-correlated $W_b = -W_f$ (Fig. 6, right) which leads to $\rho_b = \rho_f = \rho_{bf}/4$ and $\rho_{bf}^+ = 0$.

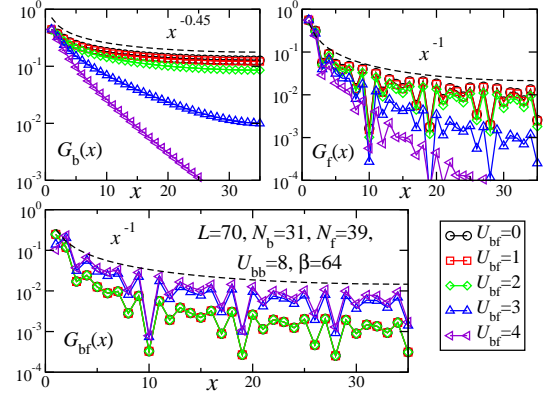


FIG. 5: Green functions for several U_{bf} . At low interaction, there are superfluid bosons and mostly free fermions (Luttinger liquids). At large interaction $U_{bf} > 3$, the system enters the PSDW regime, individual G_b and G_f decay exponentially while G_{bf} remains quasi long ranged.

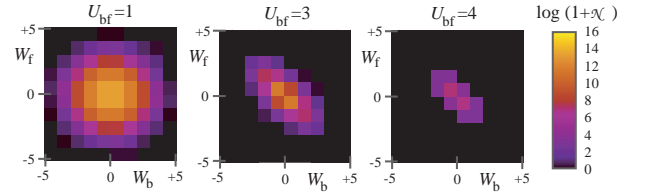


FIG. 6: Histograms of the winding numbers $\mathcal{N}(W_b, W_f)$. Same parameters as in Fig. 5. In a low interaction Luttinger liquid phase ($U_{bf} = 1$) W_b and W_f are not correlated and \mathcal{N} is isotropic (left panel). With increasing U_{bf} the winding numbers become correlated (middle panel), while in the PSDW phase ($U_{bf} = 4$), \mathcal{N} is strongly anisotropic and only allows the cases where $W_b = -W_f$ (right panel).

Along the z axis, one defines a spin correlation function $C_{psdw}(x) = \langle \sigma_i^z \sigma_{i+x}^z \rangle$. Depending on the value of J_z , the system favors antiferromagnetic (AF), for $U_{bf} < U_{bb}$, or ferromagnetic (FM), for $U_{bf} > U_{bb}$, correlations along the z -axis. For $U_{bf} > 2U_{bb}$, $|J_z| > |J_{xy}|$, the dominant correlations are ferromagnetic along the z -axis which leads to phase separation for the bosons and fermions. In all other cases, the xy term is dominant, *i.e.*, G_{bf} is the correlation function that has the slowest decay.

We concentrate on this latter case. In the AF regime along the z direction, we observe the characteristic oscillations around zero, the FM correlations decreasing much more rapidly than the AF ones (see Fig. 7). The presence of defects in the AF due to the imbalance between the populations of up and down spins leads to oscillations with beating where $C_{psdw}(x)$ behaves like $\cos(2\pi N_f x/L)$ multiplied by a power law envelope. Density correlation functions exhibit similar beating oscillations, reminiscent of the solitonic excitations observed in the extended Hubbard model [15]. The commensurate oscillations in $\cos(\pi x)$ are recovered only for $N_f = N_b = L/2$ (see Fig. 7).

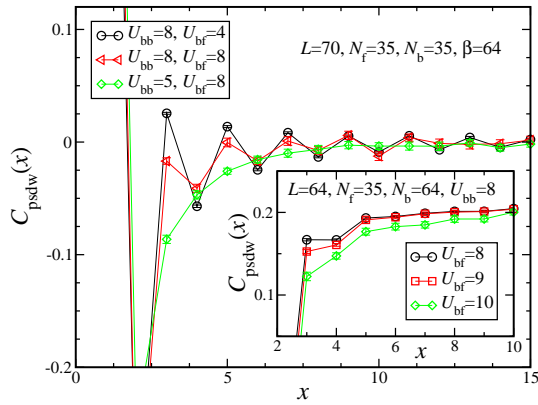


FIG. 7: Pseudo spin correlation function $C_{\text{psdw}}(x)$ in the case $N_f = N_b = L/2$ for the AF (circles), pure- xy (triangles) and FM (diamonds) regimes. Inset: $C_{\text{psdw}}(x)$ in the CSF phase for different values of U_{bf} . The AF signal decreases as expected.

On the contrary, in the FM regime, we see no sign of oscillations and observe only a slow FM relaxation. For the special case where $J_z = 0$ ($U_{\text{bf}} = U_{\text{bb}}$) the system is mapped on a pure xy pseudo-spin Hamiltonian. The AF and FM correlation functions are expected to decay with the same power law [16] and we observe the combined effect of both types of correlation (see Fig. 7).

In the SFb phase we have already seen that xy correlations are present (Fig. 4). It is more difficult to observe the PSDW correlations along the z axis. To obtain the SFb phase, one needs $U_{\text{bf}} > U_{\text{bb}}$ for the Mott phase to be destroyed. This means that the filled layer is in the FM regime. However, it is difficult to distinguish the FM signal due to the filled layer from the signal due to the superfluid boson density-density correlations which are expected to show some kind of short range relaxation. On the contrary, an AF signal would be due to the filled layer only, but should be small because we are in the region where the dominant effects are FM. We observe such a weak AF signal with a decreasing amplitude when U_{bf} increases, as expected (Fig. 7, inset).

Finally the interpretation of the SFb as composed of superfluid bosons on a filled layer in a pseudo-spin phase is partly supported by our data. We observe, as expected, that the leading correlations are the bosonic Green functions followed by the composite Green function. We also found that the measure of the pseudo-spins correlations along z are consistent with the PSDW phase. However, the decay of the fermionic Green function is algebraic which is consistent with the non-dominant PSDW correlations. The present algorithm gives access to one- and two-body correlation functions and topological information via the winding numbers. It does not give information about other N -point correlation functions or what are the dominant correlations.

In conclusion, we have studied the effect of adding fermions on a boson Mott insulator and varying the in-

teraction strength between fermions and bosons. We observed that, when the Mott insulator is destroyed, the system enters a superfluid phase where the movement of bosons and fermions is correlated. The similarities between this phase and a previously observed pseudo-spin phase led us to describe it, approximately, as a phase displaying simultaneously traditional superfluidity and PSDW.

Even in non symmetric cases, where the number of bosons and fermions is not equal, it is possible to observe some of the characteristics of the original pseudo-spin phase as long as interactions are large. These results lead us to conclude that anticorrelated motion of bosons and fermions is a robust property and appears generally in strongly interacting mixtures of bosons and fermions.

The authors thank U. Schollwöck, B. Svistunov, and M. Troyer for useful discussions. We acknowledge financial support from a grant from the CNRS (France) PICS 18796 and from the Swiss National Science Foundation. Part of the calculations were carried out on the Hreidar-cluster at ETH Zurich.

-
- [1] M. Greiner, O. Mandel, T. Esslinger, T.W. Hänsch, and I. Bloch Nature **415** 39 (2002).
 - [2] J.E. Lye, L. Fallani, M. Modugno, D.S. Wiersma, C. Fort, and M. Inguscio Phys. Rev. Lett. **95**, 070401 (2005).
D. Clément, A.F. Varón, M. Hugbart, J.A. Retter, P. Bouyer, L. Sanchez-Palencia, D.M. Gangardt, G.V. Shlyapnikov, and A. Aspect, Phys. Rev. Lett. **95**, 170409 (2005).
 - [3] F. Schreck, L. Khaykovich, K. L. Corwin, G. Ferrari, T. Bourdel, J. Cubizolles, and C. Salomon, Phys. Rev. Lett. **87**, 080403 (2001). Z. Hadzibabic, S. Gupta, C.A. Stan, C.H. Schunck, M.W. Zwierlein, K. Dieckmann, and W. Ketterle, Phys. Rev. Lett. **91**, 160401 (2003).
 - [4] M.W. Zwierlein, C.H. Schunck, A. Schirotzek, W. Ketterle, Nature **442**, 54 (2006).
 - [5] K.Günter, T. Stöferle, H. Moritz, M. Köhl, and T. Esslinger, Phys. Rev. Lett. **96**, 180402 (2006). S. Ospelkaus, C. Ospelkaus, O. Wille, M. Succo, P. Ernst, K. Sengstock, and K. Bongs Phys. Rev. Lett. **96**, 180403 (2006).
 - [6] A.B. Kuklov and B.V. Svistunov, Phys. Rev. Lett. **90**, 100401 (2003).
 - [7] M. Lewenstein, L. Santos, M.A. Baranov, and H. Fehrmann, Phys. Rev. Lett. **92**, 050401 (2004).
 - [8] L. Mathey, D.W. Wang, W. Hofstetter, M.D. Lukin, and E. Demler, Phys. Rev. Lett. **93**, 120404 (2004); L. Mathey and D.W. Wang, Phys. Rev. A **75**, 013612 (2007).
 - [9] P. Sengupta and L.P. Pryadko cond-mat/0512241 (2005).
 - [10] L. Pollet, M. Troyer, K. Van Houcke, and S.M.A. Rombouts, Phys. Rev. Lett. **96**, 190402 (2006).
 - [11] L. Pollet, C. Kollath, U. Schollwöck, and M. Troyer, cond-mat/0609604.021602(R) (2006).
 - [12] S.M.A. Rombouts, K. Van Houcke, and L. Pollet,

- Phys. Rev. Lett. **96**, 180603 (2006). K. Van Houcke, S.M.A. Rombouts, and L. Pollet, Phys. Rev. E **73**, 056703 (2006).
- [13] L. Pollet, Ph. D. Thesis, Universiteit Gent (2005). See <http://www.nustruct.ugent.be/thesislode.pdf>
- [14] These two regions are essentially the same as the two Luttinger's liquid regions (LLa and LLb) found in [10]
- [15] F. Hébert, G.G. Batrouni, and R.T. Scalettar, Phys. Rev. A **71**, 063609 (2005), cond-mat/0412037.
- [16] T. Giamarchi, *Quantum Physics in One Dimension*, Oxford (2004).